

Theory of the Temperature and Doping dependence of the Hall effect in a model with X-ray edge singularities in $d = \infty$

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We explain the anomalous features in the Hall data observed experimentally in the "normal" state of the high- T_c superconductors. We show that a consistent treatment of the local spin fluctuations in a model with x-ray edge singularities in $d = \infty$ reproduces the temperature (T) and the doping dependence (x) of the Hall constant R_H as well as the Hall angle in the normal state. The model has also been invoked to justify the marginal Fermi liquid (MFL) behavior, and provides the first consistent explanation of the Hall anomalies for a non-Fermi liquid in $d = \infty$.

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I. INTRODUCTION

The discovery of high- T_c superconductors in Cu-O based compounds has led to an upsurge of theoretical work concerning the unusual normal state properties of these materials, which appear not to conform to the framework of the Landau Fermi liquid theory [1, 2].

A way of unifying the diverse anomalies observed in experiment was proposed by Varma and coworkers [2], who suggested a phenomenological ansatz for the spectrum of charge and spin fluctuations. For low frequencies $\omega \ll v_F q$ this marginal-Fermi-liquid (MFL) ansatz is

$$\text{Im}\chi_{\rho,\sigma}(\omega) \sim \begin{cases} -\rho(0)\frac{\omega}{T}, & \omega \ll T, \\ -\rho(0), & T \ll \omega \ll \omega_c \end{cases} \quad (1)$$

where ω_c is a cut-off energy. The s.p. self-energy $\Sigma(\omega) \sim \omega \ln \omega \pm i|\omega|$, as a consequence of (1), and this reconciles the unusual normal state anomalies with the existence of the Luttinger Fermi surface.

As emphasized in [2], the singularities in (1) are in the frequency dependence; the momentum dependence is assumed smooth. The exact solution of the Falicov-Kimball model (FKM) in $d = \infty$, [3] where local fluctuations are treated exactly, has been shown to lead to the above spectrum near half-filling, and to a Fermi liquid phase at farther fillings. Furthermore, if these singularities do not depend on any special symmetries which are lost in the lattice problem, they are likely to survive in the lattice problem.

Varma et al. [2, 4] have solved a multiband Hubbard model within the impurity approximation to obtain the MFL form for the local susceptibilities. However, the MFL theory has not been able to account for the T and doping (x) dependence of the Hall constant R_H . Thus, the reconciliation of the Hall anomalies within the MFL hypothesis is clearly an open issue of current interest.

The tomographic Luttinger liquid-based model of Anderson and Ong provides a consistent explanation of the

anomalous features seen in the d.c as well as a.c Hall effect [5]. It is, however, based on an extension of 1d ideas to the 2d case; such an extension is a hotly debated issue, and there is no rigorous proof yet, inspite of intense efforts [6].

The calculation of the Hall constant for strongly correlated metals is especially hard to describe. It involves the computation of the conductivity tensor to first order in the magnetic field. This involves the rather hard problem of computing a three-point function. In addition, the calculation of the vertex corrections for strongly interacting lattice fermion models is a formidable technical problem that has not been attempted. The above reasons make it imperative to develop techniques where some of the difficulties maybe circumvented without sacrificing essential correlation effects.

The unusual T and x dependence of the Hall effect in the high- T_c s has been recognised to be a striking anomaly of the normal state, and cannot be understood within conventional Fermi liquid ideas [7-10]. In conventional metals, it is rare [8] to observe a T -dependence of R_H above a fraction (0.2 to 0.4) of the Debye temperature Θ_D . However, in the hole-doped cuprates, the Hall coefficient (with \mathbf{B} along \mathbf{c}) shows a decrease with increasing T upto room temperature, going roughly like $1/(T + C)$, where C is a constant. Suppression of superconductivity by doping with impurities or by moving away from optimal doping suppresses the T -dependence of R_H . There is no effect of phonons, in contrast to the situation in normal metals. The Hall angle $\cot\theta_H$ goes like $\alpha T^2 + \beta(x)$ [8]. The persistence of these anomalies to a rather high temperature precludes scattering mechanisms involving phonons [10] or due to anisotropic Fermi surfaces [11].

In this paper, we examine the behavior of the Hall coefficient R_H as well as the Hall angle $\cot\theta_H$ by an exact treatment of the local spin fluctuations in the uniform phase of the FKM, which exhibits x-ray edge (XRE) singularities in $d = \infty$. Our calculation presents a consistent explanation of the experimentally observed Hall anomalies, and is, we believe, the first microscopic calculation of the Hall anomalies for a non-FL metal in $d = \infty$.

II. THEORETICAL FRAMEWORK: MODEL AND LOCAL SPECTRAL DENSITY

In what follows, we consider the Falicov-Kimball model as an effective model describing the electronic degrees of freedom in the CuO_2 layers in the cuprate SCs. The Falicov-Kimball model in 2d in the large U limit is defined by,

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + h.c.) + U \sum_i n_{ic} n_{id} - \mu \sum_i (n_{ic} + n_{id}) \quad (2)$$

In this model, t and U should be understood as effective parameters which are determined by comparison of the low-energy spectra of (2) with that of a more realistic three-band model [2]. The proposed FKM bears some similarity to the effective model of ref. [2]. In ref.[2], the authors started with a full three band Hubbard model involving the complete local structure of a unit Cu-O cell embedded within the 2d square Cu-O plane. In the strong correlation limit the low lying eigenstates were retained, and the resulting hamiltonian was transformed to essentially the FKM (with $U = \infty$ in our case). Another justification comes from the proposal of Anderson [1], who suggests that the non-FL anomalies in the normal state of cuprate SCs arises from effects akin to the orthogonality catastrophe in the x-ray edge problem. As remarked above, it is unclear whether the 2d Hubbard model can exhibit these phenomena. It is, nevertheless important to separate the effects coming from the x-ray edge-like physics from those arising due to low dimensionality. This enables us to separate out the effects of bandstructure (like van-Hove singularities) and investigate the extent to which strong local correlations (which are treated exactly in $d = \infty$) are responsible for the anomalous normal state behaviors.

We are able to address the first issue in this paper, since the FKM explicitly shows the x-ray edge (XRE) behavior in $d = \infty$. We mention that such calculations for the Hubbard model in $d = \infty$ have been carried out by two groups [12, 13], both of whom obtain a crossover to a Fermi liquid (FL) below a certain crossover scale T_{coh} . This is not surprising in view of the fact that the one-band Hubbard model in $d = \infty$ always has a FL paramagnetic metallic phase [14]. In contrast, the metallic state of the FKM near half-filling is a non-FL, with a crossover to a FL at higher dopings [15].

We have solved the FKM exactly in the $d = \infty$ limit by an equation-of-motion technique [15]; this reproduces exactly the known exact solution of this model in this limit [15]. In what follows, we compute the conductivity tensor exactly in $d = \infty$; this is because of the remarkable fact that the vertex corrections to the conductivity vanish identically [16] in $d = \infty$. This simplifying feature is what makes the calculation of the conductivities and of the Hall effect exact in this limit.

We have solved the lattice model exactly in $d = \infty$. Since the authors of ref.[2] solve an impurity model, they require fine-tuning of parameters to reach the critical point. Since we perform a lattice calculation exact in $d = \infty$, the critical behavior survives for a finite range of filling, as the authors of ref. [2] anticipate. In this FKM [2,15], the d holes are immobile. This means that $[n_{id}, H] = 0 \forall i$; hence, the model has an exact local $U(1)$ symmetry. We notice that the model eqn (2) is different from the usual Hubbard model, which has a global $U(1)$ symmetry associated with *total* fermion number conservation. We show below that the system develops extra singularities in a magnetic field, in addition to those implied by the XRE physics, of a form necessary to explain the anomalous Hall data.

The exact computation of the local c-fermion single particle propagator in $d = \infty$ follows the steps in ref. [10], and yields (for a Lorentzian unperturbed DOS $\rho_o(z) = (\Delta/\pi)(z^2 + \Delta^2)^{-1}$, Δ being the effective bandwidth in the unperturbed problem)

$$G_{ii}^c(i\omega_\ell) = \frac{1}{2\pi} \left[\frac{1 - n_d}{i\omega_\ell + i\Delta \text{sgn}\omega_\ell} + \frac{n_d}{i\omega_\ell - U + i\Delta \text{sgn}\omega_\ell} \right] \quad (3)$$

with the self-energy

$$\Sigma_c(i\omega_\ell) = U n_d + \frac{U^2 n_d (1 - n_d)}{i\omega_\ell - U(1 - n_d) + i\Delta \text{sgn}\omega_\ell} . \quad (4)$$

Also, it is easily seen that

$$\langle \langle n_{id} c_i; c_i^\dagger \rangle \rangle_{i\omega_\ell} = \frac{n_d}{2\pi} \frac{1}{i\omega_\ell - U + i\Delta \text{sgn}\omega_\ell} . \quad (5)$$

The s.p. and the two-particle local spectral densities are

$$\rho_c(\omega) = \frac{\Delta}{2\pi^2} \left[\frac{1 - n_d}{\omega^2 + \Delta^2} + \frac{n_d}{(\omega - U)^2 + \Delta^2} \right] \quad (6)$$

and

$$\rho^{(2)}(\omega) = \frac{\Delta}{2\pi^2} \frac{n_d}{(\omega - U)^2 + \Delta^2} . \quad (7)$$

From eqns (6) and (7), it is clear that the low-energy spectrum is a superposition of s.p. and two-particle states, leading to a breakdown of Landau's Fermi liquid theory.

III. COMPUTATION OF THE HALL EFFECT

The computation of the Hall constant involves evaluation of the conductivity tensor $\sigma_{\alpha\beta}(\omega = 0)$. In the $d = \infty$ approximation the transport coefficients do not involve the vertex corrections [16] and the dc conductivity is given by

$$\sigma_{xx}(0) = c_{xx} \int d\epsilon \rho_0(\epsilon) \int d\omega A^2(\epsilon, \omega) \beta \frac{\text{sech}^2(\beta\omega/2)}{4} \quad (8)$$

where $c_{xx} = e^2\pi/(d\hbar a_0)$, a_0 is the lattice spacing, $\rho_0(\epsilon)$ is the bare (lorentzian) density of states (DOS) and $A(\epsilon, \omega) = -(1/\pi)\text{Im}[\omega + \mu - \epsilon - \Sigma(\omega)]^{-1}$ is the s.p. spectral function. The Hall conductivity is given by [17]

$$\sigma_{xy}(0) = Bc_{xy} \int d\epsilon \rho_0(\epsilon) \epsilon \int d\omega A^3(\epsilon, \omega) \beta \frac{\text{sech}^2(\beta\omega/2)}{4} \quad (9)$$

where $c_{xy} = |e|^3\pi^2 a_0/3d^2\hbar^2$. The Hall constant and the Hall angle are then given by $R_H = \sigma_{xy}(0)/B\sigma_{xx}^2(0)$ and $\cot\theta_H = \sigma_{xx}(0)/B\sigma_{xy}(0)$. We see that the Hall constant enters to zeroth order in $1/d$ inspite of the conductivities entering to order $1/d$ and $1/d^2$ respectively (see eqns above).

In the remainder, we use the spectral density eqn (6) to compute the Hall constant and the Hall angle as a function of the doping concentration x and temperature T . We work with $U/\Delta = 4.0$, a value representative of the strongly correlated case that also allows us to compare our results with those obtained for the Hubbard model with the same parameters by Majumdar et al. [12]. We choose values of the hole concentration to illustrate the qualitatively different regimes; (1) $x = 0.1$, $x = 0.2$, to describe the *optimally* doped regime, and (2) $x = 0.32$, the *overdoped* regime. We will further work in the quantum paramagnetic case ($n_c = n_d$ [18]). Thus, our results should apply best to these cases where there is no remnant of long-range order. To treat the underdoped case, one has to consider short-range AFM fluctuations, which grow as one approaches the limit of half-filling. This would require us to consider possible ground states with broken symmetries, and is beyond the scope of this work. In addition to antiferromagnetic fluctuations, the effects of *disorder* are also dominant in the underdoped regime, and this requires a reanalysis with the inclusion of disorder effects in a MFL [19].

The local spectral density of the model exhibits a two subband structure with the characteristic transfer of spectral weight of excitations from the *upper* to the *lower* Hubbard band upon hole doping. The inset to FIG.4 shows the evolution of the chemical potential μ determined from the eqn $n = 1 - x = n_d + \int_{-\infty}^{\mu} \rho_c(\omega)d\omega$ with hole doping. It is important, for what follows, to emphasize the fact that μ is in the region of the overlapping s.p. and two-particle spectral densities (see eqns (6)-(7)) for case (1), while it has clearly moved out of this region into the s.p. part of the spectral density for the overdoped case (2).

IV. RESULTS AND DISCUSSION

In FIG.1, we show the field-free inplane resistivity $\rho_{xx}(T)$ as well as the Hall constant R_H for the cases (1)

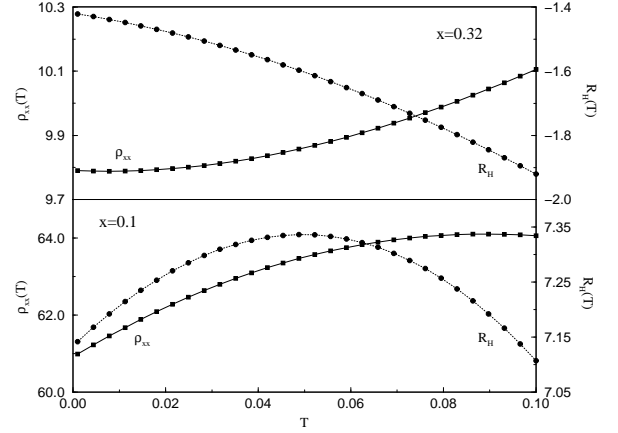


FIG. 1. Resistivity $\rho_{xx}(T)$ and $R_H(T)$ as a function of T for two values of doping ($x_1 = 0.32$ (upper) & $x_2 = 0.1$ (lower Panel)). Notice the change of slope in the resistivity from sublinear to quadratic as also a sign change in $R_H(T)$ with increasing x .

& (2) above. We also show the T -dependence of the Hall angle for the case (1) in FIG.2. In FIG.3 we show the striking linear-in- T dependence of $\rho_{xx}(T)$ for $x = 0.2$ over a wide temperature scale. This linear behavior, observed near optimal doping, has been regarded as one of the signals of the non-Fermi liquid metallic normal state of the cuprate SCs. Remarkably, we see that the essential features of the T -dependence of R_H as well as $\cot\theta_H$ are reproduced in qualitative agreement with experimental results [7-10]. More remarkably, in the FIG.4, we see that R_H as a function of doping changes sign and becomes (for hole doping) negative at around the x_c corresponding to the MFL to FL crossover. The inplane resistivity also goes quadratically with T for $x = 0.32 > x_c$, (FIG.1) revealing the doping-induced crossover to a FL. Note however, that our approach does not allow us to study the evolution of these quantities close to half-filling as remarked above.

We reproduce qualitatively the correct T -dependence for R_H as well as $\cot\theta_H$ observed in the optimally doped case. R_H goes roughly like $1/T$ at intermediate T , followed by a tendency to saturate as T_c is approached from above. The Hall angle $\cot\theta_H$ follows a T^2 dependence over a wide temperature scale. This means that the Hall conductivity σ_H goes like $1/T^3$, again consistent with observations [8]. The magnetoconductance $\Delta\sigma_{xx} \simeq \sigma_{xx}(\omega_c\tau_H)^2$, and so goes like $1/T^5$ (see the ref.[20] and references therein). The fact that the $1/\tau_H$ goes like T^2 leads also to a microscopic justification for the idea of two relaxation times in the normal state of cuprate SCs. The connection to Anderson's proposal of two relaxation rates in the cuprate materials is suggestive, and our calculation shows that the anomalies are linked to the XRE-like physics inherent in the FKM

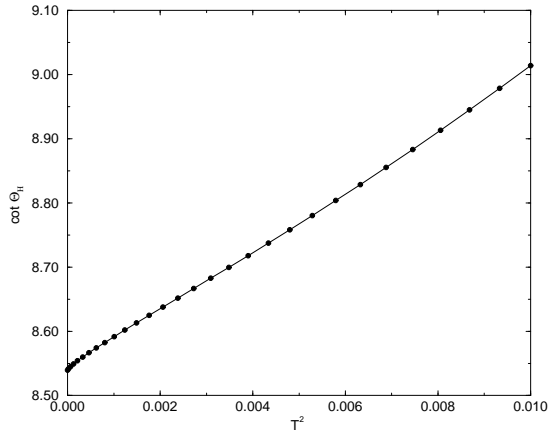


FIG. 2. Hall angle $\cot\theta_H(T)$ at $x = 0.1$. It goes as $g(T) = aT^2 + b$ over a wide temperature range.

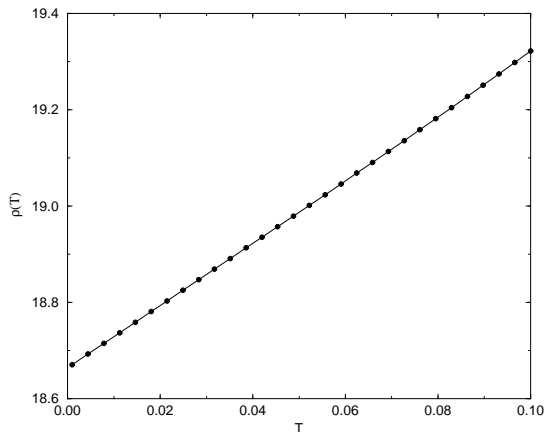


FIG. 3. Resistivity $\rho_{xx}(T)$ for $x = 0.2$. The clean linear behavior over a very wide temperature scale is clear.

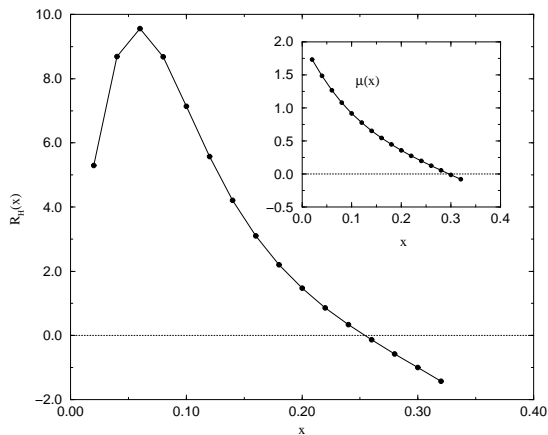


FIG. 4. Hall constant $R_H(x)$ as a function of x . It changes sign at around the x_c corresponding to the MFL-FL crossover with doping.

in $d = \infty$. The XRE model in any dimension can be bosonized [1] to a Tomonaga-Luttinger-like model on a half-line, leading to asymptotic spin-charge separation. Thus, our results represent a higher-dimensional realization of Anderson's ideas.

Earlier studies have developed this idea within a phenomenological framework using the Boltzmann equation [20]. The skew-scattering phenomenology requires near perfect particle-hole symmetry [21], while the other approach [20] invokes two scattering processes that are either even or odd under the charge-conjugation operator. Anderson [5] has provided a consistent explanation of the Hall anomalies within the framework of the tomographic Luttinger liquid hypothesis. However, it has not so far been shown conclusively [6,22,23] that the Luttinger liquid concept can be extended to two dimensions. Recently, Mahesh et al. [24] have computed the T and x dependence of R_H by numerical diagonalization of the one-band Hubbard model on finite-sized clusters. They were able to account for the anomalous behavior of R_H . We have provided an alternative explanation for the magnetotransport anomalies within the $d = \infty$ approximation, which for the effective Falicov-Kimball model also leads to a non-Fermi liquid near $n = 1$.

It is interesting to compare our results with those obtained for the Hubbard model by Majumdar et al. [12], who studied the Hubbard model with a weak next-nearest-neighbor (n.n.n) hopping strength t' in $d = \infty$ using the iterated perturbation theory away from half-filling. They studied the T -dependence of the usual Hall constant, as well as that of the infinite-frequency Hall constant R_H^* [25]. This latter quantity does not depend on the low-energy structure in the s.p. spectrum, but measures only the effect of high-energy processes. Majumdar et al. found, interestingly enough, that the T -dependence of R_H^* , rather than that of R_H , mimics the experimentally observed behavior. While this result can be taken as evidence, along with indications from other probes [26], of the importance of local fluctuations, it is known that the Hubbard model, with or without n.n.n hopping, always yields a $T = 0$ paramagnetic Fermi liquid metallic phase in $d = \infty$ [27]. A natural explanation of the observation made in [12] arises within our calculation. In contrast to the situation in the Hubbard model, the spectrum at low energies in the FKM is scale-invariant, there is no coherent FL-like feature at low- T , and the high-energy incoherent features in the spectral density are pulled down to low energy. Close to half-filling, the chemical potential μ is pinned in the region where the spectrum is a superposition of the low-energy s.p. and the high-energy two-particle states, and so the transport is dominated by anomalous high-energy scattering processes. With increasing deviation from the $n = 1$ case, μ shifts out of this region (inset of the FIG.4) into the s.p.-dominated part of the spectrum, leading to the emergence of a more conventional behavior, as evidenced in the change of sign in $R_H(x)$ as a function of doping (FIG.4).

A problem with the calculations presented here is the finite $T = 0$ intercept in $\rho_{xx}(T)$ as well as $\cot\theta_H(T)$. The resistivity $\rho_{xx}(T) = \rho_0 + \alpha T$ where α decreases with increasing Δ or x , while $\cot\theta_H(T) = aT^2 + b$. This is indicative of residual elastic scattering processes, resulting from the quenched d "impurities" at $T = 0$ in our calculations. This is the artifact of the $d = \infty$ limit, and finite dimensional extensions are required to remedy this situation. Physically, the effects of static disorder could lead to such effects, as seen in experiments. We have not done this here, however.

V. CONCLUSION

To conclude, we have presented the first explicit calculation of the Hall anomalies observed experimentally in the normal state of cuprate SCs. We have shown that the observed Hall anomalies as a function of temperature and doping, along with those seen in magnetotransport, can be understood simply in terms of the scale-invariant, non-FL spectrum characteristic of a model exhibiting XRE-like singularities in $d = \infty$. It has also been possible to show [3] that the exact solution of the FKM in $d = \infty$ has a non Fermi liquid (NFL) metallic phase near $n = 1$, and so our results also represent a first microscopic calculation of the Hall anomalies for a strongly correlated non-FL metal.

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